Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Random-Phase Approximation with Chiral NN+3N Interactions



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Clusters
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Introduction

In theoretical nuclear structure physics one tries to explain the properties of nuclei that have already been measured by experiment, as well as to predict the yet unknown attributes of, e.g., exotic nuclei. The theoretical interpretation of known qualities serves the purpose of validating the accuracy of the respective theories and models, while the prediction of so far unexplored characteristics is important to obtain information about the properties of nuclei that are not – or only with great effort – accessible to an experimental investigation. Additionally, theoretical predictions also provide information for the design of future experiments.

Methods

The randomphase approximation (RPA) provides a framework, which allows for the investigation of excited collective states and their transition strengths. While other methods such as the no-core shell model (NCSM) or the coupled-cluster theory may yield results which are superior from a methodological perspective to those from RPA, this improved accuracy comes at great computational cost, limiting such calculations to low- and medium-mass nuclei. The RPA on the other hand allows for a computationally reasonable description of excited collective states and their structure for all nuclei across the nuclear chart. Thus, the RPA provides a theoretical approach to a series of observables which are experimentally well accessible but cannot be reached via ab initio methods such as the NCSM. Our research focuses on different electric multipole transitions, which are also accessible to an experimental analysis.

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Results

For a long time, the only RPA calculations that have been conducted were on the level of two-body (2B) forces or phenomenological three-body (3B) forces. However, in recent years the advances in theoretical and computational methods have made it possible to also include full 3B forces. In our research, we extended the existing RPA code to full 3B forces, as well as to normalordered (NO) Hamiltonians for closed-shell nuclei. The input for our calculations are not phenomenological but chiral NN+3N interactions, the same ones as are used in NCSM. We were able to perform the corresponding calculations for a series of nuclei and found a significant improvement in the agreement between our theoretical results and the ones obtained from experiment. An extension of the standard RPA is the Second RPA (SRPA), which we extended to normal-ordered 3B forces. Here we found an even better agreement between theory and experiment. In the past, the theoretical predictions for transitions often were at much higher energies the experimental results. Thanks to these advances, in many cases the theoretical predictions are now in reasonable agreement with experiment, validating both the underlying interaction as well as the RPA.

Outlook

However, this increased accuracy of our predictions comes at a great computational cost. We already put a lot of effort into the development our models as well as our codes to ensure that they use as little resources as possible. Still, for larger systems the runtime, especially for models such as the SRPA, increases tremendously, even when using parallelization (OpenMP and MPI). In order to be able to improve the predictions of systems we already investigated and to push to even larger ones, we need the continued support of high performance computers.

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